Naval Oceanographic
and Atmospheric
Research Laboratory

Technical Note 207
December 1991

AD-A246 146

Three-Dimensional Ocean Thermal Structure (TOTS) Software Module

Software Requirements Specification

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Abstract

The Tactical Environmental Support System (TESS(3)) is gearing up to receive and process digital visible and infrared imagery from the civilian and military polar orbiter meteorological satellites. Real-time data from the National Oceanic and Atmospheric Administration (NOAA) Advanced Very High Resolution Radiometer (AVHRR) and the Defense Meteorological Satellite Program (DMSP) Operational Linescan System (OLS) sensors will be used for a variety of applications. The Three dimensional Ocean Thermal Structure (TOTS) software module described here uses the infrared imagery to derive ocean front and eddy positions and then incorporates feature models of the eddies and fronts to create synthetic profiles of temperature versus depth. These observations fill a critical gap in our knowledge of the real-time thermal field. The ability to combine this information with all in situ reports and generate a 3-d volume of temperature and sound speed is detailed for subsequent input to acoustic models.

Acknowledgments

Early efforts to create the TOTS module were helped considerably by the work of Jim Cummings (FNOC, the developer of the *OTIS 2.1 code) and recent efforts of John Harding,* Doug May and Gerald Stephenson of (NOARL). Documentation in this technical note was streamlined with the help of Mark Boston (NAVOCEANO). This work was supported by the Chief of Naval Operations (OP-096), the Space and Naval Warfare Systems Command Satellite Applications and Techniques Program, Program Element No.0603704N, CDR Peter Ranelli, Program Manager.

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1.0 SCOPE

1.1 IDENTIFICATION

This Software Requirements Specification (SRS) establishes the requirements for the Computer Software Configuration Item (CSCI) identified as the Three-dimensional Ocean Thermal Structure (TOTS) version 1.0.

2.0 DOCUMENT OVERVIEW

TOTS is a software module targeted for implementation on the Tactical Environmental Support System (TESS(3)) to provide ocean temperature, salinity and sound speed fields in support of Fleet ocean/acoustic predictions and weapon/sensor systems. This Software Requirements Specification describes the requirements, interfaces, and capabilities of TOTS 1.0.

3.0 REQUIREMENTS

3.1 *CSCI CAPABILITY REQUIREMENTS*

The TOTS analysis, which is based on the Optimum Interpolation (OI) data assimilation technique, combines remotely sensed sea surface temperature data with other local observations (from aircraft, ships, or buoys), front and eddy maps, data provided from shore sites, and climatology to produce a three-dimensional real-time analysis of the ocean thermal structure at specified grid points within a selected area of interest.

Input data used for the TOTS analysis include: front and eddy maps received from shore sites and earlier TOTS runs, satellite-derived MultiChannel Sea Surface Temperatures (MCSST), subsurface temperature profiles collected by ships or aircraft using expendable bathythermographs (XBTs), and sea surface temperatures (SSTs) from ships or buoys (fixed and drifting).

In addition, several databases are used for the TOTS analysis; they are the Generalized Digital Environmental Model (GDEM) climatology developed by the Naval Oceanographic Office (NAVOCEANO), the dynamic GDEM climatology, temperature covariance data bases, regional land/sea mask, data bases for constructing synthetic temperature and salinity profiles based upon empirical orthogonal functions, and the water mass classification database.

The data analysis technique used in TOTS follows the approach of Alaka and Elvander (1972) by using climatology as the first-

guess field for the optimal interpolation analysis. In the TOTS analysis, GDEM climatology is used as the first-guess field, and anomalies between GDEM climatology and other types of data are used in the data analysis.

Modeling of mesoscale features based on the front and eddy maps is utilized in TOTS to generate synthetic observations. The front and eddy maps prepared by the Navy's operational oceanography centers are used to help determine the location and shape of ocean features.

The MCSST data are used in two ways. First, MCSST images are incorporated with the front and eddy files received from shore sites to produce more accurate front and eddy maps. Second, the values of MCSST are entered as observations into the TOTS analysis.

Other temperature data used in the data analysis include surface and profile temperature data (i.e., SSTs and XBTs).

TOTS 1.0 consists of six major computer software components (CSCs) as shown in Figure 1. They are the Preliminary Data Preparation (PDP), Profile Climatology Preparation (PCP), Synthetic Profile Generation (SPG), Observation Classification and Anomaly Generation (OCAG), and Observation Selection, Sort, and SST averaging (OSSSA), and Optimal Interpolation Analysis (OIA).

3.1.1 CSC Preliminary Data Preparation (PDP)

The PDP prepares data obtained from different sources for the TOTS analysis. The first function of the PDP is to edit and create a file containing information about ocean mesoscale features through the Interactive Front and Eddy Editor (IFEE). The second function of this CSC is to assure data obtained from different sources occur within specific time frames, area limits, and resolution in order to assemble the most appropriate observations for analysis. The flow chart for the PDP is shown in Figure 2.

The data used for the PDP are front and eddy maps received from shore sites, previous maps from earlier TOTS runs if available, the image product from the Sea Surface Temperature Analysis and Composite (SSTAC) module, and the file containing all observations.

In the IFEE, operators may combine the SST image generated in the SSTAC with shore-site front and eddy maps and other data interactively to create an upgraded front and eddy map. This map identifies the surface location of high thermal gradients associated with mesoscale features in frontal regions.

In order to make the processing more efficient, observations in the original data file are checked against both an operator-specified time window and geographic boundary limits. Data outside

TOTS 1.0

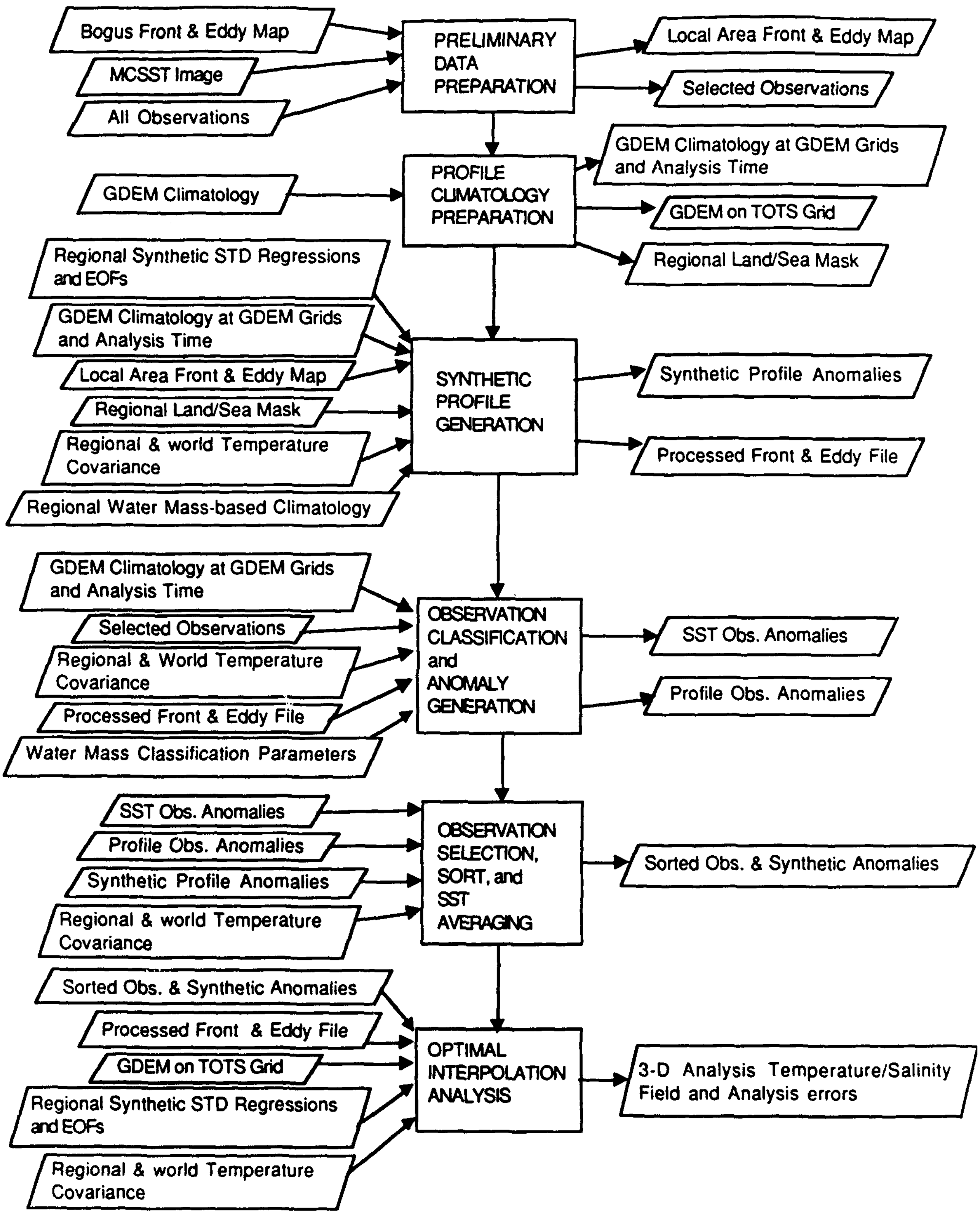

Figure 1 TOTS 1.0

Preliminary Data Preparation (PDP) Function

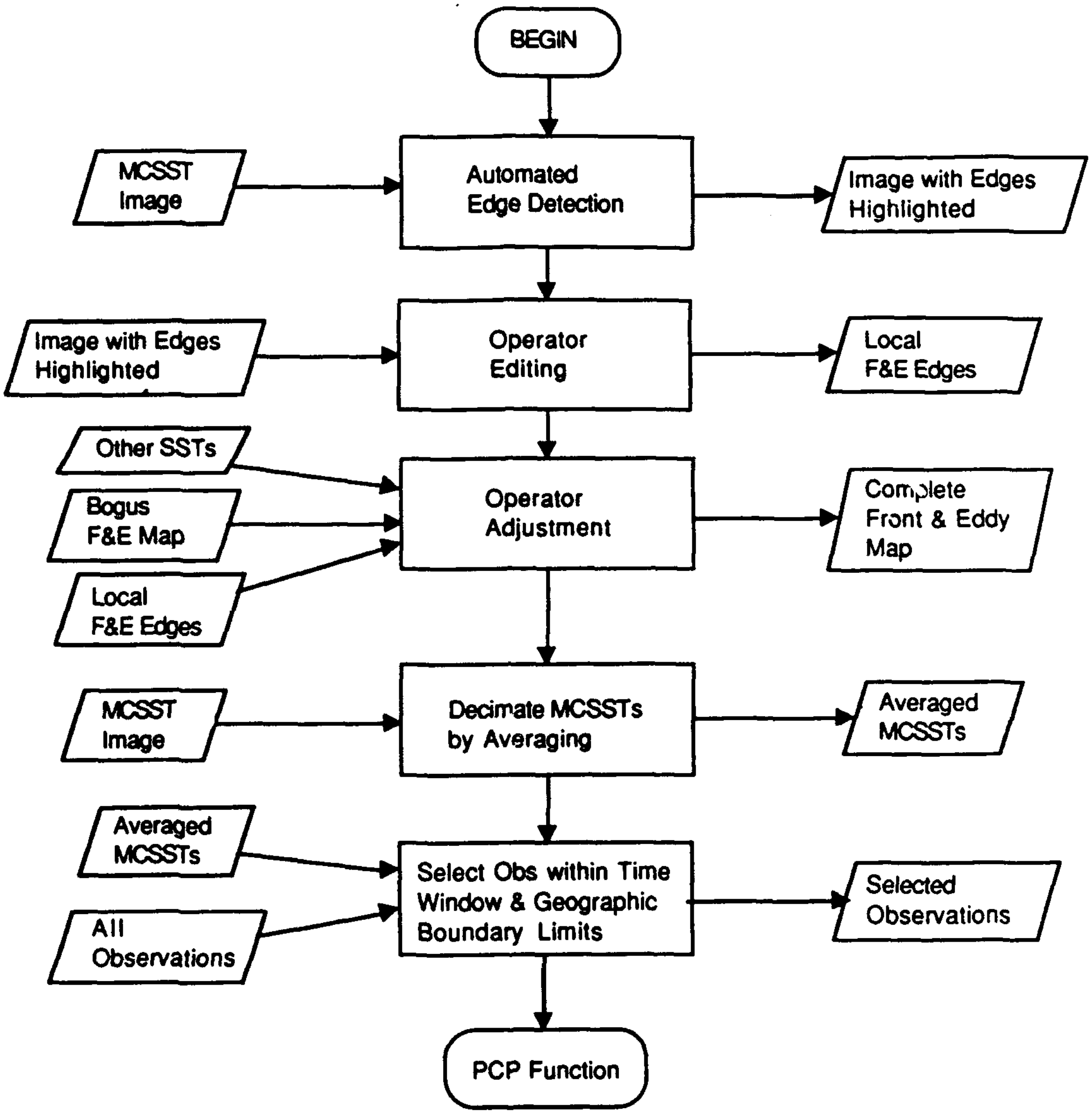

Figure 2 PDP

the time and spatial limits are excluded from later processing.

Typically, large amounts of MCSST data will be received by TOTS. The number of these satellite observations must be limited to insure reasonable processing time. Operators may specify parameters for a grid mesh to cover the analysis region. Then, all MCSSTs within each grid cell are averaged to produce a single MCSST for the grid cell.

The outputs from the PDP are a front and eddy file and a file containing observations from different sources in which MCSSTs are selected to represent their original large database.

3.1.2 CSC Profile Climatology Preparation (PCP)

The PCP reads and prepares the GDEM climatology database for rapid access by the following CSCs. The flow chart for the PCP is shown in Figure 3.

Data used in the PCP are the GDEM climatology database.

Time and spatial interpolations are used to obtain climatology profiles at the specific analysis times and desired locations. GDEM values are available on a 0.5 degree geographic grid at seasonal intervals at depths greater than 400 m, and at monthly intervals in the upper 400 m. Then, the depth of sea bottom (land/sea mask) at each analysis grid point is approximated to the depth level where the GDEM temperature is not defined.

The output of the PCP contains two sets of climatology profiles at the analysis time: one contains profiles at each of the original climatology database locations and the other contains profiles at each position of the analysis grid. The former is used for obtaining climatology profiles at the observation locations through spatial interpolation in the following CSCs. The latter will be used for determining climatology profiles at regular grid points in the last CSC. In addition, there is an output file containing a regional land/sea mask.

3.1.3 CSC Synthetic Profile Generation (SPG)

The SPG creates synthetic temperature and salinity profiles based on feature models. Feature modeling is a means to more fully utilize the limited in situ and remotely sensed data by supplementing the data with our knowledge of the typical three-dimensional structure of fronts and eddies. However, feature models are not generic, but are regionally dependent. TOTS 1.0 contains feature models for the Gulf Stream. Feature models for the Kuroshio and GINSEA are presently under development. If no feature model is available for a particular area being analyzed, this component will not be executed and the analysis will continue without using feature models (i.e., no synthetic profile is

Profile Climatology Preparation (PCP) Function

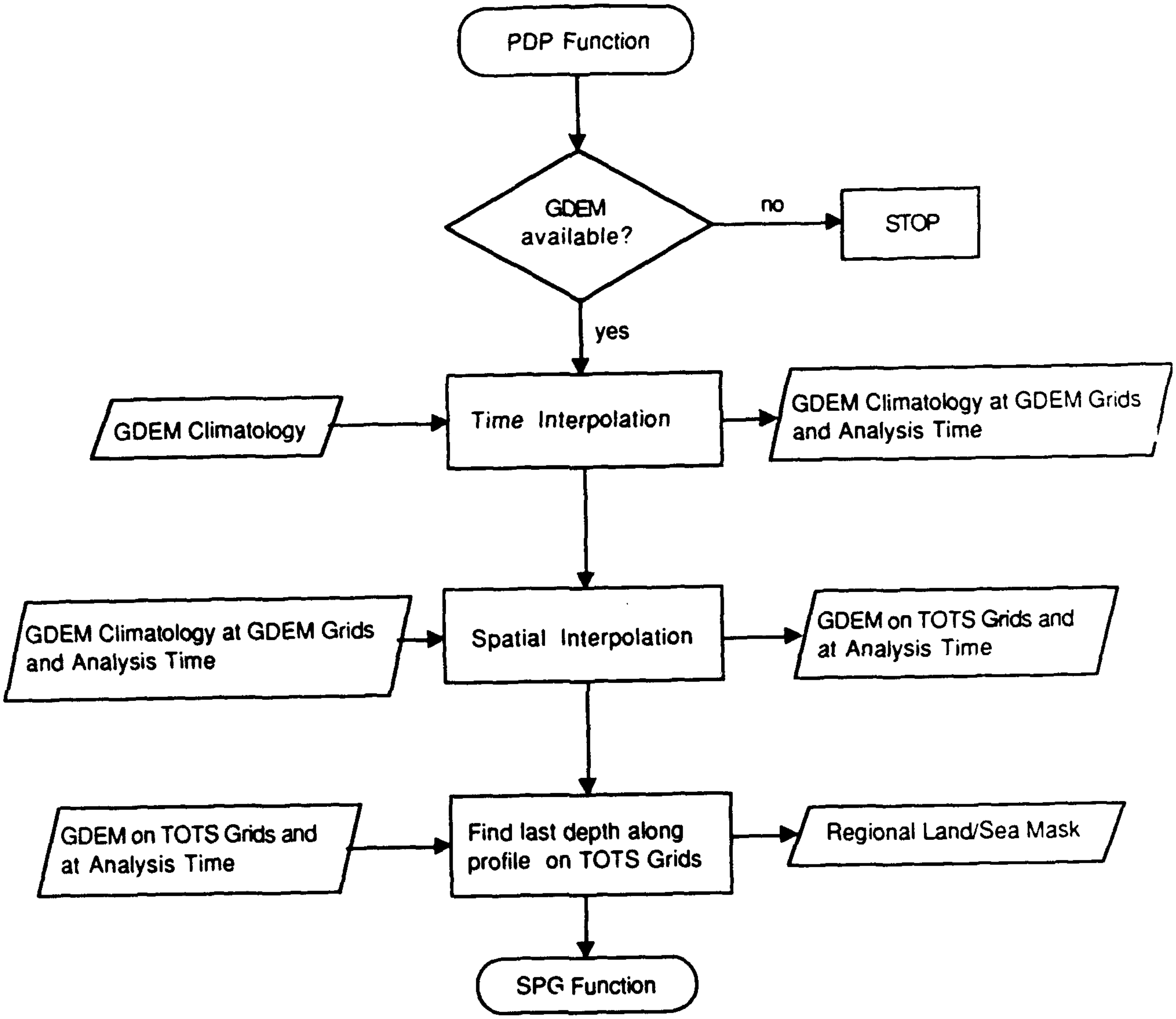

Figure 3 PCP

generated for data analysis). Figure 4 shows the flow chart for the SPG.

Inputs used for the SPG include the front and eddy file, GDEM climatology at the GDEM grid and analysis time, regional land/sea mask, dynamic GDEM climatology, data bases for constructing synthetic temperature and salinity profiles based upon empirical orthogonal functions (EOFs), and temperature covariance data bases.

After the front and eddy file is read and processed, frontal paths are identified, and the eddy parameters (size, center location, orientation) are determined. Then, the frontal paths and eddy parameters are used in conjunction with specific ocean feature models to generate synthetic observations.

The sampling scheme for synthetic profile locations near a front works on original operator-defined grid points. Whether a grid point is sampled is based on its water mass classification and distance from the front. At each sampled point, the orthogonal distance to the front and the orthogonal crossing point on the frontal path are calculated. The expected temperature difference across the front is calculated by bilinear interpolation of a water mass based temperature climatology to the orthogonal crossing point. The front model then transitions the temperature difference across the front to the analysis location forming the frontal gradient based upon the computed width and slope of the front.

For each eddy, sampling points are selected. The points are selected on two ellipses, at 1/3 and 2/3 the radius of the ring. On each ellipse, the samples are selected every 45 degrees on the inner ellipse and every 22.5 degrees on the outer ellipse. The model integrates the gradient-current relationship using an assumed solid body rotation velocity profile for the eddy to give an estimate of absolute dynamic topography at each point within the ring. The subsurface thermal structure at each sampling point is then estimated using EOFs and regression relationships that relate surface dynamic height and, if available, SST, to the vertical structure of temperature in the analysis region. The synthetic salinity profiles at sampling points are obtained from the same techniques.

For both fronts and eddies, a synthetic observation anomaly profile is calculated as synthetic observation minus climatology. The resultant synthetic anomaly profiles from the front and eddy feature models are added to the observational database for the data assimilation.

The outputs of the SPG are a processed front file that contains frontal path information, a processed eddy file that contains eddy parameters, and a file containing synthetic temperature and salinity anomaly profiles.

3.1.4 CSC Observation Classification and Anomaly Generation

Synthetic Profile Generation (SPG) Funtcion

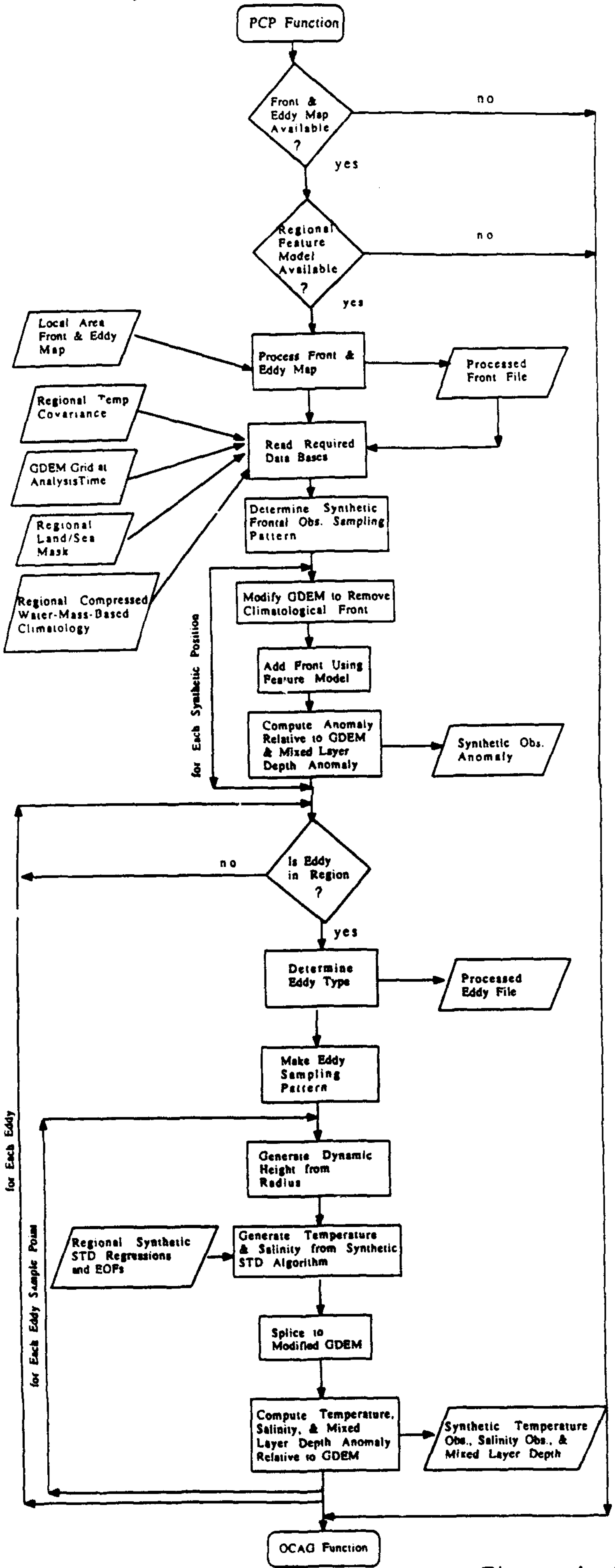

Figure 4 SPG

(OCAG)

The OCAG reads all observations, classifies them based on statistical water mass analysis, and merges BTs below the last sampled depth. The flow chart for the OCAG is shown in Figure 5.

The inputs for the OCAG include the file containing all observations selected by the PDP, water mass classification parameters, the covariance database, processed front and eddy files, and the GDEM climatology at the GDEM grid and analysis time. Observations are classified based primarily on the parameters stored in the water mass classification database.

At the beginning, the OCAG reads all observations and extracts the GDEM climatology at observation locations. Then, the water mass type for each observation is determined as described in the following.

Based on the observation time, the mean temperature and standard deviations for different water masses are extracted from the corresponding monthly data set. There are seven standard depth levels in the monthly data sets. The probability that the observation belongs to a water mass type can be calculated for each water mass and each water depth by assuming that the temperature distribution is normal. For each observation and each depth, the water mass type with the highest calculated probability is selected. The probability is set to zero at standard depths greater than the profile depth. For a profile observation, this results in a most probable water type at each of the seven standard depths. Then, the water mass type is set to the water mass type with the highest probability in the upper 150 meters. For a surface observation, there is only one most possible water mass type (i.e., at the surface).

Next, the processed front and eddy file is used to determine whether the observation is on the north side or south side of the front. If the observation located on the north side of the stream is classified as Sargasso Water, its water mass type is changed to a "warm core ring" classification code. Similarly, if the observation located on the south of the stream is classified as Slope Water, it is assigned a "cold core ring" code.

After observation classification, profile observations are extended from the last sampled depth to the bottom by merging to the GDEM climatology. Then, each observation anomaly is computed by subtracting the observation from GDEM at the observation location.

The outputs for the OCAG are two anomaly files: one with surface observations (SST) and the other with profile observations (XBT).

3.1.5 CSC Observation Selection, Sort, and SST Averaging (OSSSA)

Observation Classification and Anomaly Generation (OCAG) Function

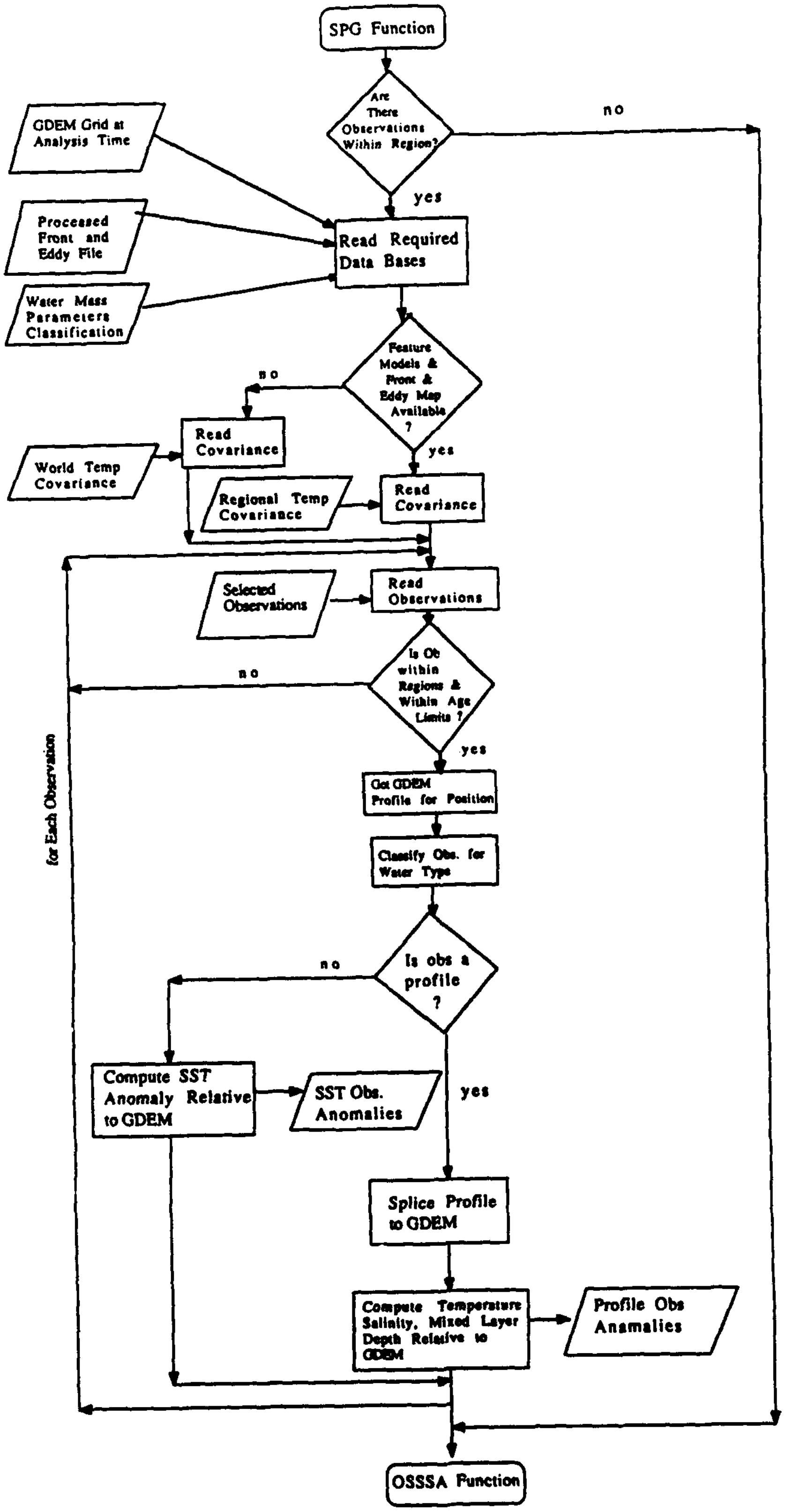

Figure 5 OCAG

The OSSSA selects data within specified age limits and determines their location bin number. Dense SST data are averaged to form a representative observation called "super obs." All observed and synthetic anomalies are sorted by bin number. Figure 6 shows the flow chart for the OSSSA.

The input files used for the OSSSA include the surface observation (SST) anomaly file, subsurface (XBT) observation anomaly file, synthetic observation anomaly file, and covariance database. The three anomaly files contain all the data to be used in the data assimilation.

The age of each bathy (XBT and synthetic) or SST observation anomaly is checked against the retention age and time decorrelation factor, and the data quality flag is checked against maximum quality limit. Data exceeding these limits are excluded from the following analysis.

In order for the data analysis to work efficiently, the observational data must be highly organized. Thus, in the OSSSA, data are sorted into data bins. The bin sizes are equal to five times the grid mesh lengths in both the longitude and latitude directions. The observational data points within a bin are assigned the same bin number. Then, in the following CSC, only data within bins close to the analysis point will be searched to select highly correlated data. Data within bins far away from the analysis point are excluded from the search and selection. This process reduces processing time.

The MCSST and buoy data are reduced by spatially averaging observations within a operator-specified number of correlation length scales and within the same water mass to form "super obs." The data are weighted according to the age of observations (i.e., the more recent data are more heavily weighted).

The output from the OSSSA is the file containing sorted observation and synthetic anomalies, which is ready for data assimilation in the next CSC.

3.1.6 CSC Optimal Interpolation Analysis (OIA)

The OIA uses optimum interpolation techniques to combine selected observations from various sources with climatology to produce a gridded three-dimensional analysis of current ocean thermal structure within the area of interest. The flow chart for the OIA is shown in Figure 7.

The inputs of the OIA are the sorted observation and synthetic anomalies from the previous CSC, temperature covariance databases, climatology on the operator-specified analysis time and grid (from surface to bottom), processed front and eddy files, and databases for constructing salinity profiles based upon empirical orthogonal

Observation Selection, Sort, and SST Averaging (OSSSA) Function

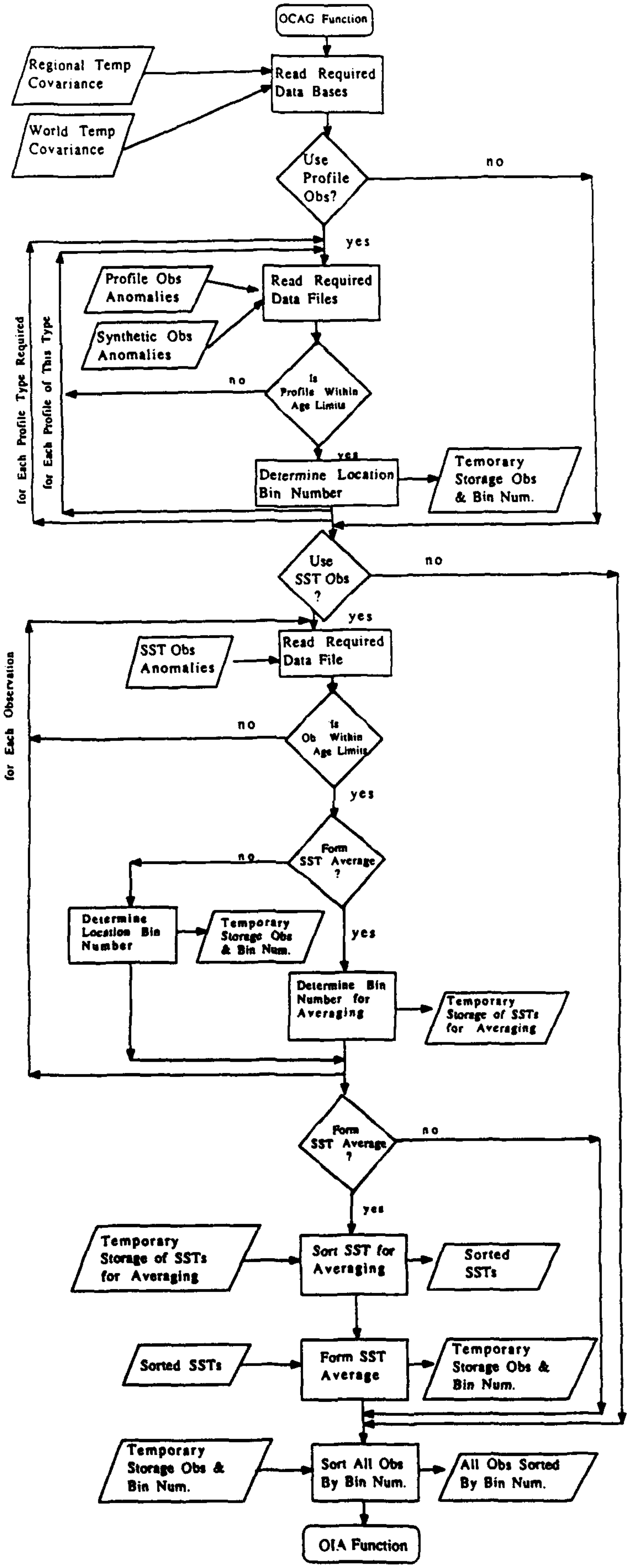

Figure 6 OSSSA

Optimal Interpolation Analysis (OIA) Function

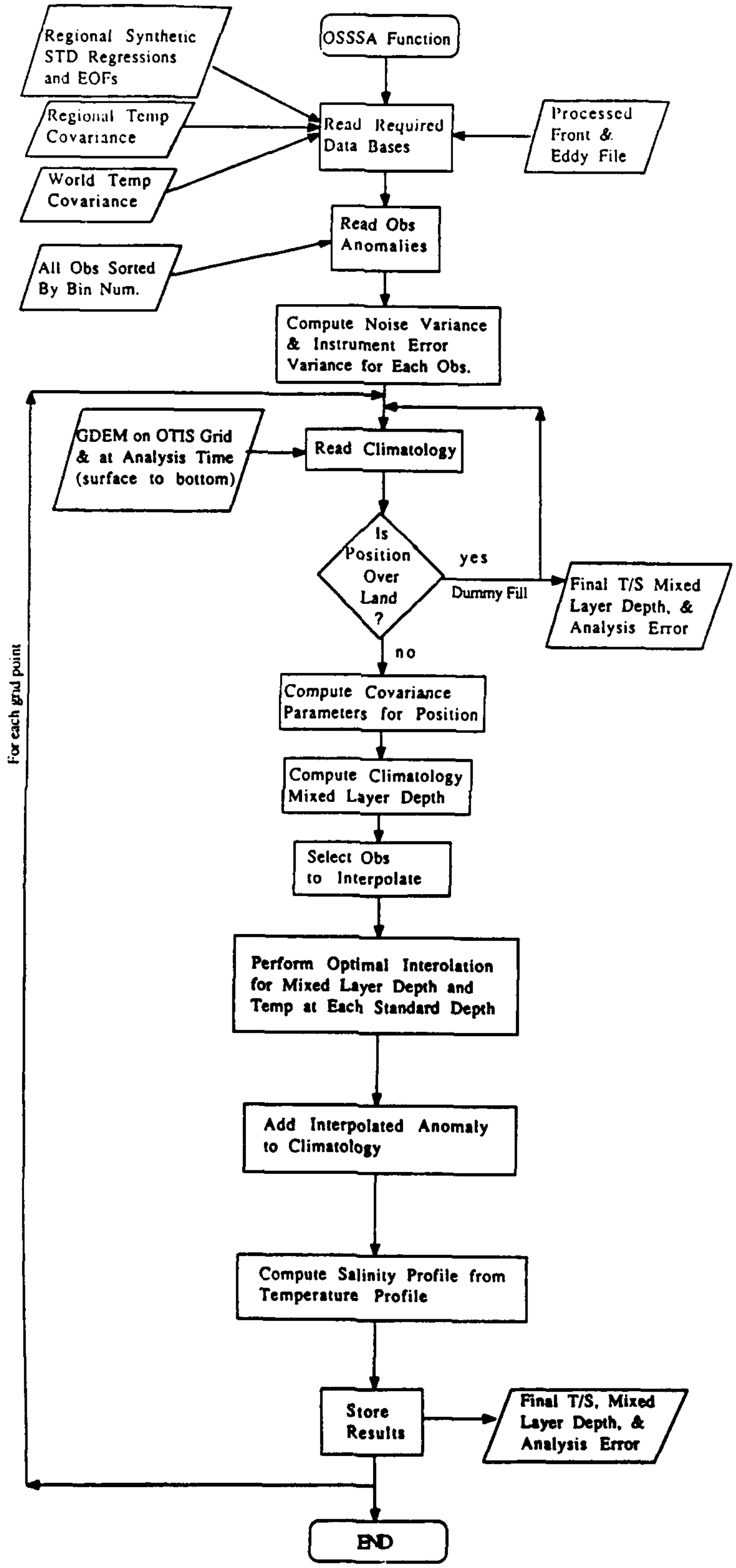

Figure 7 OIA

functions (EOFs).

The analysis proceeds point-by-point through its horizontal grid, producing a complete profile of analyzed anomalies at specified depths from the surface to the sea bottom.

At each analysis grid point, a maximum of 24 observations (i.e., 12 real observations and 12 synthetic observations) from the sorted data file are selected for the optimal interpolation The selection of data for a grid point analysis starts with the determination of data bins from which data will be selected. The number of data bins selected depends on data density and on the grid point's water mass decorrelation length scales. Data bins immediately surrounding the analysis location are searched first. If these contain insufficient data, then the search radius is extended, and the next outer layer of bins are selected and so on until the decorrelation scales are exceeded. All selected observations with high observation-to-grid correlations are retained if the correlations among observations are not too high (say, 1.0). This ensures that the analysis will contain the most independent information and that the covariance matrix will be diagonally dominant.

The optimum interpolation methodology requires the specification of several statistical parameters. Each data type (i.e., satellite MCSSTs, XBTs, ship SSTs, buoy SSTs, etc.) is assigned an associated instrument error variance for the measurement system providing the observation. The remaining statistical parameters required by the OI are the noise-to-signal ratio and the temporal and spatial decorrelation scales.

Upon completion of the optimal interpolation analysis, an analyzed temperature profile will be available at each analysis grid point. The associated analysis error will be provided for each analysis location and depth.

After the temperature profiles in the analysis area have been determined, the salinity profiles at the same grid point locations are derived. Salinity is computed directly from the temperature profiles using the EOFs and regression relationships (which relate salinity to temperature) in regions where these relationships are available. Salinity is set to climatology (GDEM) in regions where EOF relationships are not available.

3.2 CSCI INTERNAL INTERFACES

As shown in Figure 1, TOTS 1.0 consists of six CSCs. At the beginning of TOTS 1.0, the PDP (flow chart is shown in Figure 2) reads the initialization file and prepares a file containing all observations and a file containing the front and eddy information. Then, the PCP (Figure 3) prepares climatology as the first-guess field. According to the front and eddy map prepared by the PDP, the SPG (Figure 4) generates synthetic profiles through feature

models. Since climatology is used as the first guess field in the TOTS analysis, the synthetic profile anomaly relative to climatology (prepared by the PCP) is computed. The OCAG (Figure 5) reads the observation file prepared by the PDP. Each observation is classified based on its location and water mass type, and its anomaly relative to climatology is computed. In the OSSSA (Figure 6), the synthetic profile anomalies and observation anomalies prepared by the SPG and the OCAG are read, selected, and sorted. The file containing sorted observed and synthetic anomalies are read by the OIA (Figure 7). At each analysis grid point, several data points with high observation-to-grid correlations from the sorted data file are selected for the optimal interpolation calculations. The statistical estimates of ocean temperature with associated analysis error for all grid points are determined. Finally, the salinity profiles at analysis grid points are derived from the temperature profiles based on EOFs and regression relationship.

4.0 HUMAN PERFORMANCE REQUIREMENTS

Feature modeling provides a powerful means for supplementing the limited in situ and remotely sensed data in a manner that can reproduce the thermal structure and gradients typically associated with these features. However, feature models are only available for the North Atlantic (Gulf Stream) in TOTS 1.0. Outside this region, only GDEM climatology and measured data can be used for the data assimilation.

In order to fully reflect ocean features in the area of interest, the spacing of grid points needs to be specified with care. If the spacing is too large (i.e., coarse grids), some ocean features from the TOTS analysis may be distorted or may not be reproduced at all. Generally, many parameters are set for best performance using grid spacing of 1/5 degree in the North Atlantic and North Pacific areas. On the contrary, if the grid spacing is doubled (i.e., fine grids), the runtime for TOTS 1.0 will increase by a factor of 4.

5.0 NOTES

Abbreviations and Acronyms:

BATHY	- Bathythermograph
BT	- Bathythermograph data
CSCI	- Computer Software Configuration Item
CSC	- Computer Software Component
FNOC	- Fleet Numerical Oceanography Center
GDEM	- Generalized Digital Environmental Model
MCSST	- MultiChannel Sea Surface Temperature
NAVOCEANO	- Naval Oceanographic Office
OI	- Optimal Interpolation analysis scheme
OTIS	- Optimum Thermal Interpolation System
SRS	- Software Requirements Specification
SST	- Sea Surface Temperature
SSTAC	- Sea Surface Temperature Analysis and Composite
TESS	- Tactical Environmental Support System
TOTS	- Three-dimensional Ocean Thermal Structure
XBT	- used generically for all bathythermographs

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REPORT DOCUMENTATION PAGE

Form Approved
OBM No. 0704-0188

1. Agency Use Only *(Leave blank).*

2. Report Date.
December 1991

3. Report Type and Dates Covered.
Final

4. Title and Subtitle.
Three-Dimensional Ocean Thermal Structure (TOTS) Software Module Software Requirements Specification

5. Funding Numbers.

Program Element No.	0603704N
Project No.	0101
Task No.	100
Accession No.	DN255042

6. Author(s).
Chung-Chu Teng*, M.R. Carnes, J.D. Hawkins, and P.A. Phoebus**

7. Performing Organization Name(s) and Address(es).
Naval Oceanographic and Atmospheric Research Laboratory
Ocean Science Directorate
Stennis Space Center, Mississippi 39529-5004

8. Performing Organization Report Number.
NOARL Technical Note 207

9. Sponsoring/Monitoring Agency Name(s) and Address(es).
Space and Naval Warfare Systems Command
PMW-14
Washington, DC 20363-5100

10. Sponsoring/Monitoring Agency Report Number.
NOARL Technical Note 207

11. Supplementary Notes.
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12a. Distribution/Availability Statement.
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12b. Distribution Code.

13. Abstract *(Maximum 200 words).*

The Tactical Environmental Support System (TESS (3)) is gearing up to receive and process digital visible and infrared imagery from the civilian and military polar orbiter meteorological satellites. Real-time data from the National Oceanic and Atmospheric Administration (NOAA) Advanced Very High Resolution Radiometer (AVHRR) and the Defense Meteorological Satellite Program (DMSP) Operational Linescan System (OLS) sensors will be used for variety of applications. The Three dimensional Ocean Thermal Structure (TOTS) software module described here uses the infrared imagery to derive ocean front and eddy positions and then incorporates feature models of the eddies and fronts to create synthetic profiles of temperature versus depth. These observations fill a critical gap in our knowledge of the real-time thermal field. The ability to combine this information with all in situ reports and generate a 3-d volume of temperature and sound speed is detailed for subsequent input to acoustic models.

14. Subject Terms.
Digital Image Analyses, Remote Sensing, Data Analysis, Fronts and Eddies, Satellite Oceanography

15. Number of Pages.
21

16. Price Code.

17. Security Classification of Report.	**18. Security Classification of This Page.**	**19. Security Classification of Abstract.**	**20. Limitation of Abstract.**
Unclassified	Unclassified	Unclassified	SAR